A nonlinear quantum model of the Friedmann universe

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Abstract

A discussion is given of the quantisation of a physical system with finite degrees of freedom subject to a Hamiltonian constraint by treating time as a constrained classical variable interacting with an unconstrained quantum state. This leads to a quantisation scheme that yields a Schrödinger-type equation which is in general nonlinear in evolution. Nevertheless it is compatible with a probabilistic interpretation of quantum mechanics and in particular the construction of a Hilbert space with a Euclidean norm is possible. The new scheme is applied to the quantisation of a Friedmann universe with a massive scalar field whose dynamical behaviour is investigated numerically.

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1 Introduction

An elegant way of formulating classical particle dynamics is via an action principle that is invariant under a general change of time parameterisation. Such a formulation is called a parameterised theory. In non-relativistic particle dynamics a parametric description is obtained by regarding Newtonian time of the particle as a dynamical variable depending on a newly introduced "parameter time" [1]. As this choice is arbitrary the corresponding Lagrangian admits a symmetry under re-parameterisation of time, leading to a constraining relation called the Hamiltonian constraint. Consequently not all canonical variables (including the original Newtonian time and its conjugate momentum) can be given arbitrary initial data. Rather, the Hamiltonian constraint must be satisfied initially which will be preserved under the canonical equations of motion. This is to be expected since parameterising time cannot change physical kinematics, the apparent extra degree of freedom associated with time must be subject to a constraint.

In relativity the parameterised theory is ideally suited for formulating particle dynamics where time is treated on an equal footing with other coordinates. This is especially the case for a particle moving in a (pseudo) Riemannian geometry [2]. The canonical description of a parameterised relativistic particle is similar in structure to that of a non-relativistic particle. However the constrained Hamiltonian is now quadratic in the canonical momenta of both position and time coordinates. This is due to the (general) covariance of relativistic kinematics and can be analysed within the established methodology in classical theory. However this appears to present a number of challenges for the quantisation of a relativistic particle compatible with standard interpretations. As is well-known, a straightforward application of canonical quantisation results in a Klein-Gordon equation. Unfortunately its solutions belong to a function space with an indefinite norm and cannot be interpreted as

wavefunctions describing a probability amplitude in the usual manner. Although this difficulty can be circumvented upon "second quantisation" in the context of relativistic quantum field theory, theoretical interest remains in search for a satisfactory direct quantisation of a relativistic particle. One important reason for this is that a functional form of relativistic particle dynamics naturally arises from canonical general relativity [3]. Furthermore systems with finite degrees of freedom subject to a constrained Hamiltonian formally resembling that of relativistic particle dynamics in curved spacetime often feature in various cosmological models with or without coupled matter fields. These models are normally constructed by imposing high symmetry on spacetime geometry and matter distribution in order to gain insight into aspects of an underlying full theory. Note that in these models the "metric" refers to the (reduced) "supermetric" (of spacetime metric) and the "relativistic particle" represents a collective gravitational and matter field point.

In [4] a "square-root Hamiltonian" method was investigated in an attempt to overcome the problems mentioned with the "Klein-Gordon approach". Given a choice of time coordinate it is possible to construct a wave equation that is first order in time and possesses a "Schrödinger structure". While in some cases this structure guarantees the existence of a Hilbert space with a Euclidean norm it may suffer from other drawbacks including the violation of Hermiticity of the Hamiltonian operator if the square-root of a negative eigenvalue must be taken through a spectral analysis [5].

Motivated by these circumstances an alternative canonical type of quantisation for a physical system with finite degrees of freedom subject to a Hamiltonian constraint is considered by treating time as a constrained classical variable interacting with an unconstrained quantum state. Following a brief review of the basic parameterised theory of a non-relativistic particle in curved space and its Dirac quantisation in section 2, a new "parametric quantisation" is introduced. For non-relativistic particle dynamics, this new scheme is shown to reproduce results based on Dirac quantisation. In section 3, parametric quantisation of a relativistic particle in curved spacetime is performed for a choice of time-slicing. In this case a "nonlinear Schrödinger equation" may be derived that is locally equivalent to the full set of evolution equations from parametric quantisation under certain conditions. In section 4 the theory is applied in the context of a simple Friedmann cosmological model with the resulting equations analysed numerically. Concluding remarks are made in section 5 where some prospects for future work are also discussed.

2 Classical and quantum dynamics of a non-relativistic particle

Consider the motion of a non-relativistic particle subject to a potential in a Riemannian n-space. Denote by τ the Newtonian time and introduce the coordinates (q^α) $(0 \leq \alpha \leq n$ with $q^0 := \tau)$. The time-dependent spatial metric components are denoted by $\gamma_{ab} = \gamma_{ab}(q^\alpha) = \gamma_{ab}(q^c, \tau)$. Here and throughout Greek letters such as α, β denote spacetime indices with range $0, 1, \cdots n$, whereas Latin letters such as a, b denote spatial indices with range $1, 2, \cdots n$. The particle motion is described by the trajectory $(q^\alpha(t)) = (q^a(t), \tau(t))$ parameterised by a parameter time t. The choice of t is related to a positive function $N = N(t)$ that sets the parameterisation gauge and enters into the generic form of the Hamiltonian

$$H(N, q^\alpha, p_\alpha) = N\mathcal{H}(q^\alpha, p_\alpha) \tag{1}$$

that generates the dynamics of the particle for some $\mathcal{H}$. For a non-relativistic particle with canonical momenta $\varpi := p_0$ and p_a conjugate to τ and q^a respectively, $\mathcal{H}$ is linear in ϖ and quadratic in p_a as given by

$$\mathcal{H} = \varpi + \frac{1}{2}\gamma^{ab}p_a p_b + V \tag{2}$$

where $V(q^\alpha) = V(q^c, \tau)$ is a time-varying potential and the particle's mass has been normalised to unity. Based on an action principle using the Lagrangian

$$L = \dot{q}^\alpha p_\alpha - H \tag{3}$$

where $\dot{} = \frac{\mathrm{d}}{\mathrm{d}t}$, the equations of motion can be derived in the following canonical form:

$$\frac{\mathrm{d}q^a}{\mathrm{d}t} = N\frac{\partial \mathcal{H}}{\partial p_a}, \quad \frac{\mathrm{d}p_a}{\mathrm{d}t} = -N\frac{\partial \mathcal{H}}{\partial q^a} \tag{4}$$

$$\frac{\mathrm{d}\tau}{\mathrm{d}t} = N\frac{\partial \mathcal{H}}{\partial \varpi}, \quad \frac{\mathrm{d}\varpi}{\mathrm{d}t} = -N\frac{\partial \mathcal{H}}{\partial \tau}. \tag{5}$$

In addition the Hamiltonian constraint

$$\mathcal{H} = 0 \tag{6}$$

arises from variations with respect to N. Provided a set of initial conditions for the canonical variables q^α and p_α compatible with (6) is given, this constraint will be preserved by the evolution of the canonical variables satisfying (4) and (5) for a choice of (positive) $N(t)$. Clearly the particle trajectory is invariant under re-parameterisation: $t \to t'$, $N \to N' := \frac{\mathrm{d}t}{\mathrm{d}t'}N$.

A quantum theory of this particles may be established by applying Dirac quantisation where, in the Schrödinger picture, classical constraints are "turned into" operators that annihilate wavefunctions describing physical states. Following this procedure, the operator

$$\hat{\mathcal{H}}_D(q^a, \hat{p}_a, \tau, \hat{\varpi}) := \hat{\varpi} + \frac{1}{2}\gamma^{-\frac{1}{4}}\hat{p}_a\gamma^{\frac{1}{2}}\gamma^{ab}\hat{p}_b\gamma^{-\frac{1}{4}} + V \tag{7}$$

where $\gamma := \det(\gamma_{ab})$ is constructed by substituting $p_\alpha \to \hat{p}_\alpha := -1\frac{\partial}{\partial q^\alpha}$ in $\mathcal{H}$ and factor ordering so that the resulting term quadratic in $\hat{p}^a$ is proportional to the Laplacian operator on a wavefunction $\Psi(q^a, \tau)$ of weight $\frac{1}{2}$ with respect to the metric γ_{ab}. Such a weighting choice is very useful in simplifying mathematical expressions when dealing with the wavefunction of a quantum particle moving in a time dependent spatial metric.

On Dirac quantisation the classical constraint (6) becomes the quantum constraint

$$\hat{\mathcal{H}}_D\,\Psi = 0 \tag{8}$$

on any physical state Ψ. Although (8) does not explicitly involve the parameter time t it is natural to interpret τ as the evolution parameter for wavefunctions. To see this more clearly we may rewrite (8) in the form

$$1\frac{\partial}{\partial \tau}\Psi = \hat{\boldsymbol{\mathcal{H}}}\Psi \tag{9}$$

where

$$\hat{\boldsymbol{\mathcal{H}}} := \frac{1}{2}\gamma^{-\frac{1}{4}}\hat{p}_a\gamma^{\frac{1}{2}}\gamma^{ab}\hat{p}_b\gamma^{-\frac{1}{4}} + V \tag{10}$$

plays the role of the "true Hamiltonian" as in conventional Schrödinger equations.

By treating τ as the evolution parameter the positive-definite inner product of two wavefunctions Ψ_1 and Ψ_2 at equal time τ is naturally defined as

$$\langle \Psi_1, \Psi_2 \rangle := \int \Psi_1^* \Psi_2 \,\mathrm{d}^n q. \tag{11}$$

Using this definition the operator $\hat{\boldsymbol{\mathcal{H}}}$ is self-adjoint and the standard probabilistic interpretation of quantum mechanics applies. In particular if a wavefunction Ψ is initially normalised according to $\langle \Psi, \Psi \rangle = 1$ this normalisation will be maintained under (8) and therefore the conservation of the total probability holds.

The derivation of the non-relativistic Schrödinger equation (8) above is often regarded as support for Dirac quantisation. However it is worthy noting that this derivation crucially relies on the fact that $\mathcal{H}$ is *linear* in the momentum ϖ conjugate to the time variable τ. For a relativistic particle, this is no longer the case, since the Hamiltonian will be quadratic in all momenta instead.

It is a purpose of this paper to point out the possibility of deriving (8) based on an alternative quantisation scheme in which the substitution $\varpi \to -\imath \frac{\partial}{\partial \tau}$ is *not* made and the explicit parameter time (t) dependence will be retained. The guiding principle is that one of the dynamical variables of a parameterised system should play the role of time. In the case of non-relativistic particle dynamics, τ has been chosen to be this variable. As a time variable it is of "classical nature" but need not be treated merely as a parameter. Indeed in classical parameterised theory such a time variable is treated as a dynamical variable whose conjugate momentum is subject to a Hamiltonian constraint without changing the underlying physical degrees of freedom. In view of this we seek to formulate an analogous quantisation procedure where the selected time variable is not quantised but treated as a *constrained classical variable.* The coupling of the classical time variable with other quantised unconstrained variables described by a wavefunction will be formulated subject to certain requirements to validate essential physical interpretations. These requirements include the existence of a positive-definite norm for the Hilbert space of the wavefunctions and the reduction to (4), (5) and (6) in the classical limit.

To achieve this consider the operator

$$\hat{\mathcal{H}}(q^a, \hat{p}_a, \tau, \varpi) := \varpi + \hat{\boldsymbol{\mathcal{H}}} \tag{12}$$

where $\hat{\boldsymbol{\mathcal{H}}}$ takes the form as given in (10). The operator $\hat{\mathcal{H}}$ is constructed in the way similar to that of $\hat{\mathcal{H}}_D$ with the substitution $p_a \to \hat{p}_a = -\imath \frac{\partial}{\partial q^a}$ in $\mathcal{H}$ but τ, ϖ now remain as classical functions of t. In contrast to Dirac quantisation where $\hat{\mathcal{H}}_D$ is used in constructing a quantum constraint equation (8), the operator $\hat{\mathcal{H}}$ will be used to formulate a Schrödinger-type equation

$$\imath \frac{\partial}{\partial t} \psi = N \hat{\mathcal{H}} \psi \tag{13}$$

for a wavefunction $\psi(q^a, t)$ of weight $\frac{1}{2}$ with respect to the metric γ_{ab}. Nonetheless, like (11), the inner product of two wavefunctions ψ_1 and ψ_2 can be defined to be

$$\langle \psi_1, \psi_2 \rangle := \int \psi_1^* \psi_2 \, \mathrm{d}^n q \tag{14}$$

under which the operator $\hat{\mathcal{H}}$ is self-adjoint. It is readily seen that (13) maintains the normalisation of the wavefunction $\langle \psi, \psi \rangle$ for *any* $\tau(t), \varpi(t)$. This makes it possible to consistently impose the special normalisation $\langle \psi, \psi \rangle = 1$ and then interpret $\psi(q^a, t)$ as the probability amplitude for measurements of the particle position (q^a) on a spatial hypersurface at time $\tau(t)$. For general normalisation, the expectation value of an operator $\hat{O} = \hat{O}(q^a, \hat{p}_a, \tau, \varpi)$ may be defined as:

$$\left\langle \hat{O} \right\rangle := \frac{\left\langle \psi, \hat{O}\, \psi \right\rangle}{\langle \psi, \psi \rangle} \tag{15}$$

in a standard manner. Sometimes it is useful to denote this expectation value by $\left\langle \hat{O} \right\rangle_\psi$ to explicitly indicate that it is evaluated with respect to the wavefunction ψ. Using (13) and (15), the derivative of the expectation value $\left\langle \hat{O} \right\rangle$ with respect to the parameter time t can be shown to be

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\langle \hat{O} \right\rangle = \left\langle \frac{\partial \hat{O}}{\partial \tau} \right\rangle \frac{\mathrm{d}\tau}{\mathrm{d}t} + \left\langle \frac{\partial \hat{O}}{\partial \varpi} \right\rangle \frac{\mathrm{d}\varpi}{\mathrm{d}t} - \imath N \left\langle \left[\hat{O}, \hat{\mathcal{H}} \right] \right\rangle \tag{16}$$

where [,] denotes a commutator as usual. The succinctness of this expression benefits from the use of weight $\frac{1}{2}$ wavefunctions and their operators. Formulae (15) and (16) will now be used to construct the governing equations for $\tau(t)$ and $\varpi(t)$. Guided by canonical equations (5) the equations

$$\frac{\mathrm{d}\tau}{\mathrm{d}t} = N\left\langle \frac{\partial \hat{\mathcal{H}}}{\partial \varpi} \right\rangle, \quad \frac{\mathrm{d}\varpi}{\mathrm{d}t} = -N\left\langle \frac{\partial \hat{\mathcal{H}}}{\partial \tau} \right\rangle \tag{17}$$

are adopted in a "semi-classical" fashion to allow the coupling between variables τ, ϖ and wavefunction ψ such that the expected classical limit may be recovered. It can now be observed that, using (16), $\left\langle \hat{\mathcal{H}} \right\rangle$ is a constant of motion under (13) and (17). That is,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \hat{\mathcal{H}} \right\rangle = 0. \tag{18}$$

Therefore the condition

$$\left\langle \hat{\mathcal{H}} \right\rangle = 0 \tag{19}$$

may be consistently imposed and regarded as the quantum analogue of the classical Hamiltonian constraint (6). This condition may be considered as a restriction on the initial classical variables τ and ϖ for any given arbitrary initial wavefunction ψ.

For a non-relativistic particle the quantum description using (13), (17) and (19) is in fact equivalent to the single Schrödinger-type equation (9). To see this first note that in this case $\dot{\tau} = N$ by using (12) and (17). Adopt the gauge $N = 1$ so that we may set $\tau = t$. With this choice it is clear at once that $\psi(q^a, \tau)$ is unitarily related to $\Psi(q^a, \tau)$ satisfying (9) via

$$\Psi(q^a, \tau) = \exp\left(\imath \int^{\tau} \varpi(\tau')\mathrm{d}\tau'\right) \psi(q^a, \tau). \tag{20}$$

Given a generic classical parameterised theory, the procedure leading to equations (13), (17) and (19) will be referred to as "parametric quantisation". Although both Dirac quantisation and parametric quantisation give rise to equivalent results for non-relativistic particle dynamics, these two schemes are in general inequivalent, as will be demonstrated in the next section.

3 Parametric quantisation of a relativistic particle

Let us now consider the motion of a particle in an $(n+1)$-dimensional pseudo-Riemannian manifold $\mathcal{M}$ [6] with coordinates (q^α), $(0 \le \alpha \le n)$, in which the metric has components $\gamma_{\alpha\beta} = \gamma_{\alpha\beta}(q^\mu)$ with signature $(-, +, +, \cdots)$. The classical Hamiltonian for this particle $H(N, q^\alpha, p_\alpha) = N\mathcal{H}$ with trajectory coordinates $q^\alpha(t)$ and canonical momenta $p_\alpha(t)$ parameterised by t associated with a positive gauge function $N(t)$ subject to a potential $V(q^\mu)$ is specified by

$$\mathcal{H}(q^\alpha, p_\alpha) = \frac{1}{2}\gamma^{\alpha\beta} p_\alpha p_\beta + V. \tag{21}$$

In order to follow closely the methods in the preceding section, the manifold $\mathcal{M}$ is assumed to admit a global time foliation so that (q^α) forms a single Gaussian coordinate chart [7] in which

$$\gamma_{00} = -1, \quad \gamma_{0a} = 0. \tag{22}$$

With such a time-slicing we denote by $\tau(t) := q^0(t)$ and $\gamma := \det(\gamma_{ab})$ where $1 \le a, b \le n$ as in the non-relativistic particle case. Thus (21) becomes

$$\mathcal{H} = -\frac{1}{2}\varpi^2 + \frac{1}{2}\gamma^{ab} p_a p_b + V \tag{23}$$

which generates canonical equations of motion

$$\frac{\mathrm{d}q^a}{\mathrm{d}t} = N\frac{\partial \mathcal{H}}{\partial p_a}, \quad \frac{\mathrm{d}p_a}{\mathrm{d}t} = -N\frac{\partial \mathcal{H}}{\partial q^a} \tag{24}$$

$$\frac{\mathrm{d}\tau}{\mathrm{d}t} = N\frac{\partial \mathcal{H}}{\partial \varpi}, \quad \frac{\mathrm{d}\varpi}{\mathrm{d}t} = -N\frac{\partial \mathcal{H}}{\partial \tau} \tag{25}$$

subject to the Hamiltonian constraint

$$\mathcal{H} = 0. \tag{26}$$

Since $\mathcal{H}$ in (23) resembles (2) we now introduce the operator

$$\hat{\mathcal{H}} := -\frac{1}{2}\varpi^2 + \hat{\boldsymbol{\mathcal{H}}} \tag{27}$$

where $\hat{\boldsymbol{\mathcal{H}}}$ takes the form of (10) and is self-adjoint with respect to the inner product

$$\langle \psi_1, \psi_2 \rangle := \int \psi_1^* \psi_2 \, \mathrm{d}^n q \tag{28}$$

of any two wavefunctions $\psi_k = \psi_k(q^a, t)$ (of weight $\frac{1}{2}$) with respect to the spatial metric γ_{ab}. As in the preceding section, parametric quantisation now yields the evolution equations for the wavefunction $\psi(q^a, t)$ and constrained classical variables $\tau(t), \varpi(t)$ as follows:

$$\mathrm{i}\frac{\partial}{\partial t}\psi = N\hat{\mathcal{H}}\psi \tag{29}$$

$$\frac{\mathrm{d}\tau}{\mathrm{d}t} = N\left\langle \frac{\partial \hat{\mathcal{H}}}{\partial \varpi} \right\rangle, \quad \frac{\mathrm{d}\varpi}{\mathrm{d}t} = -N\left\langle \frac{\partial \hat{\mathcal{H}}}{\partial \tau} \right\rangle \tag{30}$$

$$\left\langle \hat{\mathcal{H}} \right\rangle = 0 \tag{31}$$

where the definition of expectation values follows from (15). As in the non-relativistic case, the normalisation $\langle \psi, \psi \rangle = 1$ can be consistently imposed and the interpretation of $\psi(q^a, t)$ as the probability amplitude for measurements of the particle position (q^a) on a spatial hypersurface at time $\tau(t)$ can be made.

It is also possible (at least locally) to reduce (29), (30) and (31) for the relativistic case to a single wave equation. From (23), (30) and (31) it follows that $\dot{\tau} = -N\varpi$ where

$$\varpi = \pm\sqrt{2\left\langle \hat{\boldsymbol{\mathcal{H}}} \right\rangle}. \tag{32}$$

Hence in regions where $\left\langle \hat{\boldsymbol{\mathcal{H}}} \right\rangle > 0$ and $\varpi < 0$ one can explicitly eliminate ϖ and set $t = \tau$ by choosing the gauge

$$N = -\frac{1}{\varpi} \tag{33}$$

and introducing

$$\Psi(q^a, \tau) := \exp\left(\frac{1}{2}\int^{\tau} \varpi(\tau')\mathrm{d}\tau'\right) \psi(q^a, \tau) \tag{34}$$

where $\psi(q^a, \tau)$ satisfies (29) with (33). Since $\left\langle \hat{\boldsymbol{\mathcal{H}}} \right\rangle_\psi = \left\langle \hat{\boldsymbol{\mathcal{H}}} \right\rangle_\Psi$, (29) becomes

$$\mathrm{i}\frac{\partial}{\partial \tau}\Psi = \frac{\hat{\boldsymbol{\mathcal{H}}}\,\Psi}{\sqrt{2\left\langle \hat{\boldsymbol{\mathcal{H}}} \right\rangle_\Psi}}. \tag{35}$$

We are therefore led to a nonlinear integro-partial differential equation describing the quantum evolution of a relativistic particle under a chosen time-slicing. Although nonlinear in time, (35) does not present difficulties in the probabilistic interpretation of its solutions. It follows from the scaling invariance of (35), i.e. if Ψ is a solution to (35) so is $C\Psi$ for any complex constant C and hence both Ψ and $C\Psi$ represent the same physical state [8, 9].

4 Friedmann universe with a massive scalar field

It is not hard to see that the Gaussian coordinate condition $\{\gamma_{00} = -1, \gamma_{0a} = 0\}$ used in the parametric quantisation of a relativistic particle can be extended to the condition $\{\gamma_{00} = \gamma_{00}(\tau), \gamma_{0a} = 0\}$ by changing the coordinate time $\tau \to \int^{\tau} \sqrt{-\gamma_{00}(\tau')}\, \mathrm{d}\tau'$ for some negative $\gamma_{00}(\tau)$. With this coordinate condition one can repeat the derivations of (29), (30) and (31) using the operator

$$\hat{\mathcal{H}} = \frac{1}{2}\gamma_{00}\varpi^2 + \hat{\boldsymbol{\mathcal{H}}} \tag{36}$$

with the same forms of $\hat{\boldsymbol{\mathcal{H}}}$ and inner product $\langle\,,\rangle$ as defined in (10) and (28) respectively.

This slightly generalised coordinate condition makes it easier for the application of the parametric quantisation to a simple cosmological model for $n = 1$, where a Friedmann universe filled with a massive scalar field is analysed.[1] In terms of the lapse function $N(t)$ and scale factor $R(t)$ as functions of the time coordinate t, the Robertson-Walker metric reads

$$g = -N^2 \mathrm{d}t^2 + R^2\sigma \tag{37}$$

where σ is the standard metric on the homogeneous and isotropic 3-space of constant curvature K, with $K = 1, 0, -1$ corresponding to the closed, flat and open cases respectively. The dynamics of this geometry coupled to a uniformly distributed but time-dependent scalar field $\phi(t)$ of mass m is described by the Lagrangian [4]:

$$L = -\frac{6R}{N}\dot{R}^2 + \frac{R^3}{2N}\dot{\phi}^2 - \frac{Nm^2}{2}R^3\phi^2 + 6NKR \tag{38}$$

where $\dot{} = \frac{\mathrm{d}}{\mathrm{d}t}$. The corresponding action $\int L\mathrm{d}t$ is manifestly invariant under time re-parameterisation: $t \to t'$, $N \to N' := \frac{\mathrm{d}t}{\mathrm{d}t'}N$. The scale factor R will now be chosen as the (intrinsic) time variable. Accordingly we denote by $q^0 = R, q^1 = \phi$ with the corresponding conjugate momenta given by

$$p_0 = \frac{\partial L}{\partial \dot{R}} = -\frac{12R}{N}\dot{R} =: \Pi \tag{39}$$

$$p_1 = \frac{\partial L}{\partial \dot{\phi}} = \frac{R^3}{N}\dot{\phi} =: p \tag{40}$$

where symbols Π and p have been introduced for conciseness in the subsequent discussions. It follows that the Hamiltonian $H = \dot{q}^\alpha p_\alpha - L = N\mathcal{H}$ where $\alpha = 0, 1$ with $\mathcal{H}$ having the form of (21) in terms of the nonzero metric components and potential as follows:

$$\gamma_{00} = -12R, \quad \gamma_{11} = R^3 \tag{41}$$

$$V = \frac{m^2}{2}R^3\phi^2 - 6KR. \tag{42}$$

By substituting $p \to \hat{p} := -\imath\frac{\partial}{\partial\phi}$ into $\mathcal{H}$ we obtain the operator

$$\hat{\mathcal{H}}_F := -\frac{1}{2R^3}\frac{\partial^2}{\partial\phi^2} + \frac{m^2}{2}R^3\phi^2 - \frac{\Pi^2}{24R} - 6KR \tag{43}$$

[1] Units of $c = \hbar = 16\pi G = 1$ are adopted.

which is to be applied to a wavefunction $\psi(\phi, t)$ (of weight $\frac{1}{2}$ with respect to the 1-dimensional metric $\gamma_{11} = R^3$) whose norm at any time t is given by

$$\langle \psi, \psi \rangle = \int_{-\infty}^{\infty} |\psi(\phi, t)|^2 \, \mathrm{d}\phi. \tag{44}$$

For simplicity the normalisation condition

$$\langle \psi, \psi \rangle = 1 \tag{45}$$

will be imposed on the wavefunction ψ. On parametric quantisation the evolution equations for the wavefunction ψ and constrained classical variables $R(t)$ and $\Pi(t)$ are then formulated in accordance with (29), (30) and (31) as follows:

$$\imath \frac{\partial}{\partial t} \psi = N \hat{\mathcal{H}}_F \psi \tag{46}$$

$$\frac{1}{N} \frac{\mathrm{d}R}{\mathrm{d}t} = \left\langle \frac{\partial \hat{\mathcal{H}}_F}{\partial \Pi} \right\rangle = -\frac{\Pi}{12R} \tag{47}$$

$$\frac{1}{N} \frac{\mathrm{d}\Pi}{\mathrm{d}t} = -\left\langle \frac{\partial \hat{\mathcal{H}}_F}{\partial R} \right\rangle = -\left\langle \frac{3}{2R^4} \frac{\partial^2}{\partial \phi^2} + \frac{3m^2}{2} R^2 \phi^2 \right\rangle - \frac{\Pi^2}{24R^2} + 6K \tag{48}$$

$$\left\langle \hat{\mathcal{H}}_F \right\rangle = 0. \tag{49}$$

To proceed a (time-dependent) functional basis for ψ will be chosen in order to reduce the above integro-partial differential equations into a system of nonlinear ordinary differential equations of infinite dimensions. This system may be truncated to facilitate numerical simulation. To this end consider

$$\psi_k(\phi, R) := (mR^3)^{1/4} \, \xi_k(\sqrt{mR^3} \, \phi) \tag{50}$$

for integers $k \geq 0$ where

$$\xi_k(x) := 2^{-k/2} \pi^{-1/4} (k!)^{-1/2} e^{-x^2/2} \, H_k(x) \tag{51}$$

in terms of the Hermite polynomials $H_k(x)$. The functions ψ_k satisfy the eigen equations

$$\left(-\frac{1}{2R^3} \frac{\partial^2}{\partial \phi^2} + \frac{m^2}{2} R^3 \phi^2 \right) \psi_k = m \left(k + \frac{1}{2} \right) \psi_k \tag{52}$$

and orthonormality

$$\int_{-\infty}^{\infty} \psi_j(\phi, R) \psi_k(\phi, R) \mathrm{d}\phi = \delta_{jk} \tag{53}$$

for any positive R. They are used to expand the normalised wavefunction:

$$\psi(\phi, t) = \sum_{k=0}^{\infty} c_k(t) \psi_k(\phi, R(t)) \tag{54}$$

with complex coefficients $c_k(t)$ satisfying $\sum_{k=0}^{\infty} |c_k|^2 = 1$. The time-dependence of these coefficients is to be determined by dynamics. Using the expansion (54) it follows that

$$\imath \frac{\partial \psi}{\partial t} = \left[\imath \dot{c}_k + \frac{\imath N \Pi}{16R^2} \left(\sqrt{k(k-1)} \, c_{k-2} - \sqrt{(k+2)(k+1)} \, c_{k+2} \right) \right] \psi_k \tag{55}$$

and

$$\hat{\mathcal{H}}_F \psi = \sum_{k=0}^{\infty} \left[m \left(k + \frac{1}{2} \right) - \frac{\Pi^2}{24R} - 6KR \right] c_k \psi_k. \tag{56}$$

With the aide of (52), (53), (55) and (56), we obtain the following coupled differential equations for $c_k(t)$ $(k \geq 0)$, $R(t)$ and $\Pi(t)$ by substituting (54) into (46)–(49):

$$\frac{\dot{c}_k}{N} = \imath \left[\frac{\Pi^2}{24R} + 6KR - \left(k + \frac{1}{2} \right) m \right] c_k + \frac{\Pi}{16R^2} \left[\sqrt{(k+2)(k+1)}\, c_{k+2} - \sqrt{k(k-1)}\, c_{k-2} \right] \tag{57}$$

$$\frac{\dot{R}}{N} = -\frac{\Pi}{12R} \tag{58}$$

$$\frac{\dot{\Pi}}{N} = -\sum_{k=0}^{\infty} \frac{3m}{R} \sqrt{(k+1)(k+2)}\, \Re(c_k^* c_{k+2}) - \frac{\Pi^2}{24R^2} + 6K \tag{59}$$

together with the constraint

$$\sum_{k=0}^{\infty} m \left(k + \frac{1}{2} \right) |c_k|^2 - \frac{\Pi^2}{24R} - 6KR = 0 \tag{60}$$

derived from (49), and the normalisation condition

$$\sum_{k=0}^{\infty} |c_k|^2 = 1. \tag{61}$$

Based on these equations numerical simulations are performed for different choices of the curvature parameter K to explore the dynamical behaviour of the model. With the mass of the scalar $m = 10$ and gauge $N = 1$ the initial scale factor $R(t)$ at $t = 0$ is set to 0.5. The initial wave profile $\psi(\phi, 0)$ is chosen to be gaussian by setting $c_0(0) = 1$ with $c_k(0) = 0$ for $k \geq 1$, corresponding to an initially "ground state"-like wavefunction compatible with the normalisation condition (61). The initial value for the momentum $\Pi(0)$ is then determined by solving the constraint (49) at $t = 0$ with $c_k(0), R(0)$ substituted with their initial values above. This yields two signs for $\Pi(0)$ equivalent to integrations forward or backward in time t (with a negative or positive $\Pi(0)$ respectively). With these initial data and parameters, a truncated k index range $0 \leq k \leq 60$ is found to produce numerical results with satisfactory accuracy.

For an open Friedmann universe with $K = -1$ the simulated $R(t)$, $\Pi(t)$ and $|\psi(\phi, t)|^2$ are displayed in figures 1–3 for $-0.15 \leq t \leq 3.0$. The wavefunction ψ is evaluated using the expression (50) in terms of the numerical solutions for $c_k(t)$. Figure 1 clearly exhibits an expanding universe with the scale factor R growing in t and approaching a singularity $(R \to 0)$ with decreasing t. Since $\dot{R}$ does not change the sign of $\Pi(t)$ remains negative as show in figure 2. Figure 3 shows that the probability density $|\psi|^2$ with respect to the measure $\mathrm{d}\phi$ takes the shape of a single packet. As the universe evolves this packet becomes narrower and its height seems to reduce to zero as t decreases to where $R \to 0$. Despite this, the alternative probability density $\left| R^{-\frac{3}{4}} \psi \right|^2$ (corresponding to the use of the weight 0 wavefunction $R^{-\frac{3}{4}}\psi$ with respect to the measure $R^{\frac{3}{2}}\mathrm{d}\phi$) exhibits a more steady behaviour in its evolution. As shown in figure 4 the profile of $\left| R^{-\frac{3}{4}} \psi \right|^2$ as a function of $R^{\frac{3}{2}}\phi$ remains the shape of a single packet whose width simply oscillates by either increasing t or decreasing t even to where $R \to 0$. The regular behaviour of $R^{-\frac{3}{4}}\psi$ suggests that the limiting value of this function may serve to define the initial quantum state of the Friedmann universe as $R \to 0$.

Similar behaviours for R, Π and ψ can be observed from simulation results for a flat Friedmann universe with $K = 0$. The numerical solutions for $R(t)$, $\Pi(t)$ and $|\psi(\phi, t)|^2$ for a closed Friedmann universe with $K = 1$ are displayed in figures 5–7 for $-0.23 \leq t \leq 2.27$. Singularities are encountered as $R \to 0$ at both bounds of the numerical integration as shown in figure 5. Notably in figure 2, Π changes sign when the local maximum of R takes place. Nevertheless this does not cause any problem for the evolution of the system. As in the $K = -1$ case the probability density $|\psi|^2$ with respect to the

measure dϕ has the shape of a single packet. As t approaches the bounds of integration where $R \to 0$ the height of this packet also tends to zero (figure 7) whereas $\left|R^{-\frac{3}{4}}\psi\right|^2$ as a function of $R^{\frac{3}{2}}\phi$ remains the shape of a single packet with a steadily oscillating width throughout the integration domain as shown in figure 8. This provides further support for the use the limiting value of $R^{-\frac{3}{4}}\psi$ as a function of $R^{\frac{3}{2}}\phi$ to identify the initial (or final) quantum state of the Friedmann universe as $R \to 0$.

5 Concluding remarks

A quantisation scheme for a physical system subject to a Hamiltonian constraint is presented based on canonical quantisation, nonlinear quantum mechanics, couplings between classical and quantum variables and analysis of the true degrees of freedom in geometrodynamics [5]. Motivated by the need for a clarified role played by "time" in the ongoing efforts to ultimately quantise gravity, the idea of treating time as a constrained classical variable is put forward in this paper. Instead of regarding time as an evolution parameter, the proposed idea treats it as a dynamical variable while maintaining its classical nature. It does not follow that the physical degrees of freedom will increase by giving time a dynamical status since the time variable and its canonical momentum are subject to the (quantised) Hamiltonian constraint. This does imply that if the Hamiltonian constraint only restricts the choice of classical time and its canonical momentum, then the quantum degrees of freedom can be regarded as unconstrained, thereby enabling much of the standard quantisation technique to continue to apply. Of course the issue of the preferred choice of time remains just as in the square-root Hamiltonian approach. However it is worth emphasising that the proposed parametric quantisation method is free from problems associated with taking square roots of negative eigenvalues arising from a spectral analysis. Therefore the choice of a time coordinate is less restrictive for parametric quantisation. Whether there exists a naturally preferred time variable given a classical parameterised theory or possibility of establishing equivalence for different choices of time within the framework of parametric quantisation stays unaddressed in this paper and will be considered in a later publication. Finally in extending the present work to the quantisation of gravity it is conceivable that one of the traditional functional degrees of freedom in geometrodynamics should be treated as a constrained classical variable within the framework set up by this paper. York's "extrinsic time" [10] is amongst potential candidates for such a treatment. In this respect it is of interest to compare with the approach by [11]. The progress of these further researches will be reported elsewhere.

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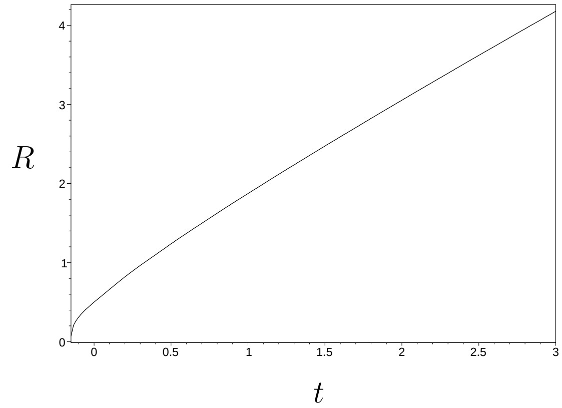

Figure 1: Simulated $R(t)$ for an open Friedmann universe ($K = -1$). An expanding universe with the scale factor R growing in t is clearly exhibited. This function approaches zero by decreasing t where the Robertson-Walker spacetime becomes singular.

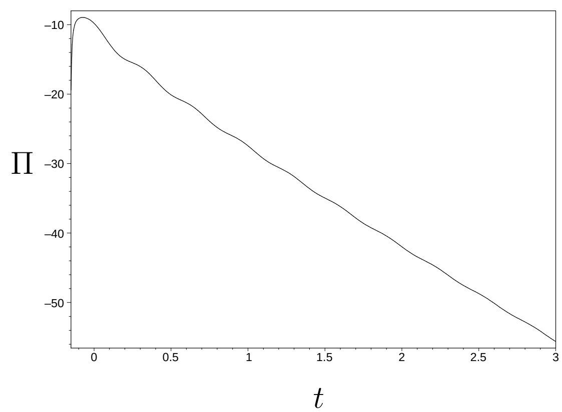

Figure 2: Simulated $\Pi(t)$ for an open Friedmann universe ($K = -1$). Since in this case $\dot{R}$ does not change the sign of $\Pi(t)$ remains negative.

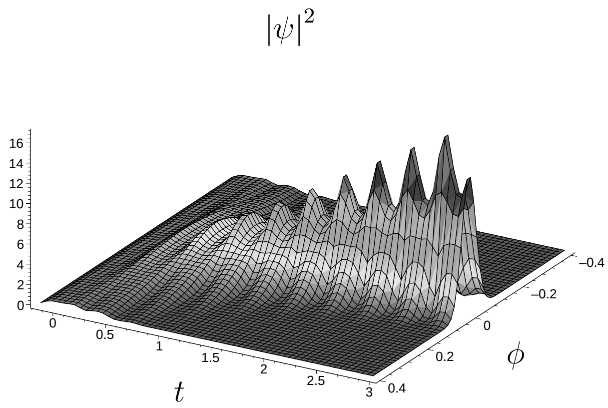

Figure 3: Behaviour of $|\psi(\phi,t)|^2$ based on simulated $\psi(\phi,t)$ for an open Friedmann universe ($K=-1$). This expression as a function of ϕ at a constant t takes the shape of a single packet. As the universe evolves this packet becomes narrower and its height reduces to zero as t decreases to where $R \to 0$.

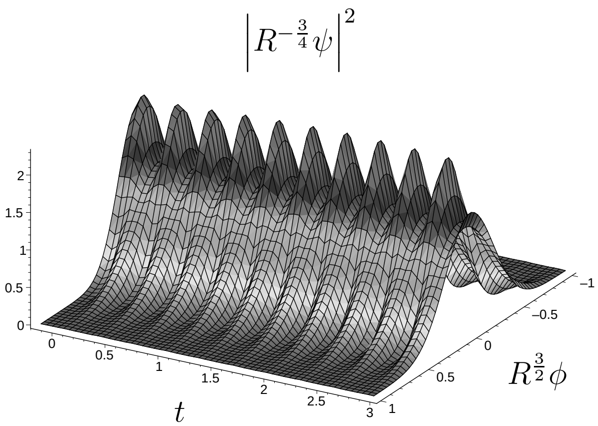

Figure 4: Behaviour of $\left|R^{-\frac{3}{4}}\psi\right|^2$ based on simulated $\psi(\phi,t)$ and $R(t)$ for an open Friedmann universe ($K=-1$). The profile of this expression as a function of $R^{\frac{3}{2}}\phi$ remains the shape of a single packet whose width simply oscillates by either increasing t or decreasing t even to where $R \to 0$.

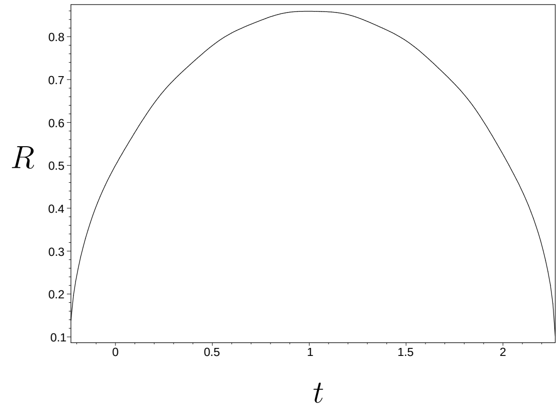

Figure 5: Simulated $R(t)$ for a closed Friedmann universe ($K = 1$). Scenarios of Big Bang and Big Crunch as $R \to$ are exhibited as in classical cases.

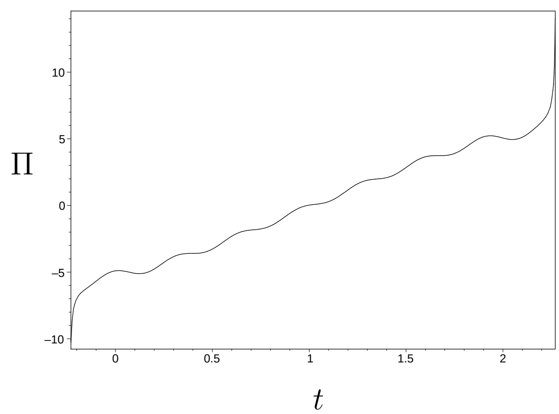

Figure 6: Simulated $\Pi(t)$ for a closed Friedmann universe ($K = 1$) This function changes sign when the local maximum of R takes place. This does not affect the continuous evolution of the system.

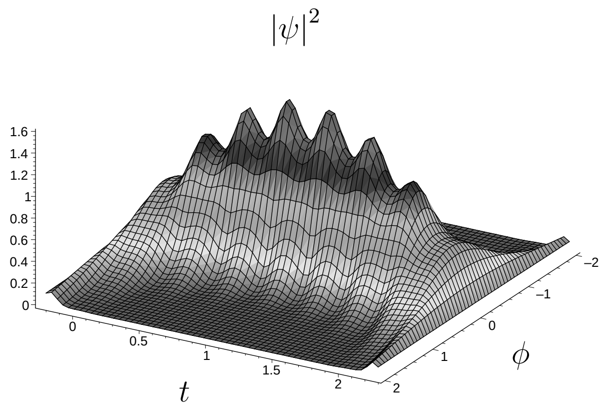

Figure 7: Behaviour of $|\psi(\phi, t)|^2$ based on simulated $\psi(\phi, t)$ for a closed Friedmann universe ($K = 1$). This expression as a function of ϕ at a constant t takes the shape of a single packet. As t approaches the bounds of integration where $R \to 0$ the height of this packet also tends to zero.

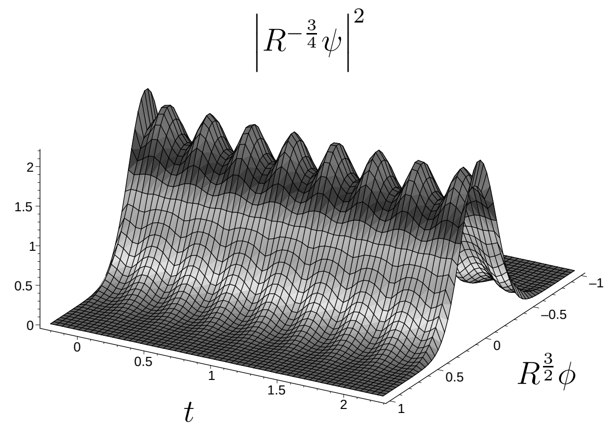

Figure 8: Behaviour of $\left|R^{-\frac{3}{4}}\psi\right|^2$ based on simulated $\psi(\phi, t)$ and $R(t)$ for a closed Friedmann universe ($K = 1$). The profile of this expression as a function of $R^{\frac{3}{2}}\phi$ remains the shape of a single packet whose width simply oscillates by either increasing t or decreasing t even to where $R \to 0$.